

Study of CdTe/CdS heterostructure by CdCl₂ heat treatment via in situ high temperature XRD

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ARTICLE INFO

Article history:

Received 27 August 2011

Received in revised form

4 November 2012

Accepted 14 November 2012

Available online 12 December 2012

Keywords:

CdTe

CdCl₂

Interdiffusion

CdS

In situ HT-XRD

ABSTRACT

A CdTe/CdS heterostructure was fabricated on Fluorine Tin Oxide glass to produce thin-film photovoltaic devices. A CdCl₂ layer was deposited onto the CdTe absorber layer and the subsequent annealing of the stack was performed in a He atmosphere. The influence of the CdCl₂-activation step on the interfaces was investigated by monitoring the phase transition of CdCl₂-heat-treated CdTe specimens during temperature ramp annealing via in situ high-temperature X-ray diffraction. X-ray Photoelectron Spectroscopy depth profiling data confirmed the interdiffusion between the CdTe and CdS layers through observation of the binding energy shifts and atomic ratio. The experimental results reveal that a compressive force, which is due to the formation of CdTe–CdCl₂ eutectic liquid phases between grains, which cause the capillary action of such liquid phases, seems to introduce a compressive strain in the plane of the film that facilitates the recrystallization process.

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1. Introduction

Post-deposition processing of polycrystalline CdTe/CdS hetero-junction solar cells with CdCl₂ has been demonstrated to improve cell efficiency by improving the electrical properties of films for photovoltaic operation [1,2]. It is well known that heat treatment with CdCl₂ is a major step in preparing high-quality CdTe/CdS solar cells [3–6]. CdCl₂ treatment has become a standard and critical process in the fabrication of high-efficiency CdTe-based photovoltaic devices, regardless of the method used for depositing the CdTe layer. The fundamental mechanism by which CdCl₂ reacts with CdTe and CdS can be expected as a similar process, despite the use of different CdCl₂ methods. That is, a chemical reaction between CdTe and CdS activated by CdCl₂ can occur, and this is the driving force for the bulk and grain-boundary interdiffusion of CdTe and CdS [7–9]. The most typical CdCl₂ methods are wet CdCl₂ treatment with a CdCl₂:CH₃OH solution and vapor CdCl₂ treatment. Wet CdCl₂ treatment, which is applied after the deposition of a CdTe absorber layer and prior to the application of a back contact, consists of soaking the CdTe films in methanol containing dissolved CdCl₂, followed by heat treatment at ~400 °C.

Optimization of the various CdCl₂ processing conditions of the CdTe/CdS layers has been studied by many research groups, but the origins of such phenomena have not yet been explained in detail.

Our previous results [10] were a study of the reaction kinetics of single CdTe thin films deposited on Corning 7059 Glass during post-deposition CdCl₂ heat treatment via in situ high-temperature X-ray diffraction (XRD) measurement. These results show that the recrystallizations of CdTe (111) and other planes do not occur simultaneously, but rather sequentially with respect to temperature. Further, the results of isothermal soaking imply that the Avrami diffusion-controlled reaction model fits well with the experimental data. This proves that the CdCl₂ diffusion process is the dominant factor in the CdTe recrystallization mechanism. In this study, additional important information was incorporated into the CdCl₂ post-deposition heat treatment of CdTe/CdS heterostructures.

2. Experimental method

In this work, we investigated the effect of CdCl₂ heat treatment on the phase transition of CdTe/CdS heterostructure thin films. In situ high-temperature XRD was used to study the kinetics and reaction mechanisms of CdTe/CdS thin films during CdCl₂ heat treatment. The CdS/CdTe layers were prepared on Fluorine Tin Oxide (FTO) glass. The CdS thin films were fabricated using a chemical bath deposition method [11]. For comparison, CdCl₂ heat treatment on CdTe/glass structures was also performed to investigate the effects of the CdS layer. CdTe thin films with a thickness of 1 μm and an average grain size of 100 nm were grown on the CdS layer using the sputtering method. The deposition conditions were

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summarized in our previous paper [10]. These deposition conditions yielded uniform single-phase CdTe films. After the deposition of the CdTe layer, the CdCl₂ treatment was performed using a solution method. For this method, the Glass/FTO/CdS/CdTe (or Glass/CdTe) specimens were coated with solid CdCl₂ of thickness 0.5 μm; this was done by pouring one drop of 1 wt% CdCl₂-CH₃OH solution on the top surface of the CdTe film, and then evaporating the CH₃OH in a drying oven at 85 °C. The high-temperature X-ray diffractometer used for this study included a Panalytical Pro-MPD θ/θ goniometer, a chamber furnace (Anton Paar HTK 16), and a PIXcel Linear Position-Sensitive Detector (LPSD) with a primary Cu-K α 1 wavelength of 1.5406 Å. The CdCl₂-deposited CdTe/CdS thin films were mounted on the heater strip using a carbon paint to improve the thermal contact between the specimens and the strip-type heater. The heater temperature was measured by a type-S thermocouple that was welded onto the bottom of the Pt strip heater, and was controlled by a PID temperature controller. First, temperature step-ramp annealing was performed to investigate the phase evolution of the samples. The temperature was ramped up in 10 °C increments at 30 °C/min, and then, XRD data were collected at a constant temperature. This sequence of step heating in 10 °C increments and XRD data collection was repeated over a temperature range of 25–550 °C in a He flowing atmosphere [10,12]. At each step, the samples were held for 6 min at the setting temperatures, 1 min for temperature stabilization and 5 min for measurement. X-ray Photoelectron Spectroscopy (XPS) analysis was conducted in a ULVAC-PHI Quanterra SXM equipped with a monochromated Al K source and a hemispherical analyzer. The energy resolution of the XPS system for high-resolution core line scans was set to 0.1 eV. The spot size was 0.4 mm. Depth profiling was performed with an argon ion source operating at a beam energy of 4000 eV and an estimated etching rate of about 1 nm/min.

3. Results and discussion

Fig. 1 shows XRD data collected for the CdTe/CdS thin films both with (a) and without (b) CdCl₂ over a temperature ramp-up range of 25–550 °C. In the case of the CdCl₂ heat treatment, as shown in Fig. 1(a), the recrystallization, grain growth, and orientation randomization occurred as a result of the step-ramp annealing, as reported previously [5]. Without CdCl₂, however, no dramatic changes in the XRD spectra were observed, as shown in Fig. 1(b).

Fig. 2 shows XRD data collected for 2θ equal to 14.2–16.2° (a), 23.2–24.2° (b), and 38.2–40.2° (c) for CdCl₂-treated CdTe/CdS samples, and 23.2–24.2° (d) for a sample without CdCl₂ treatment.

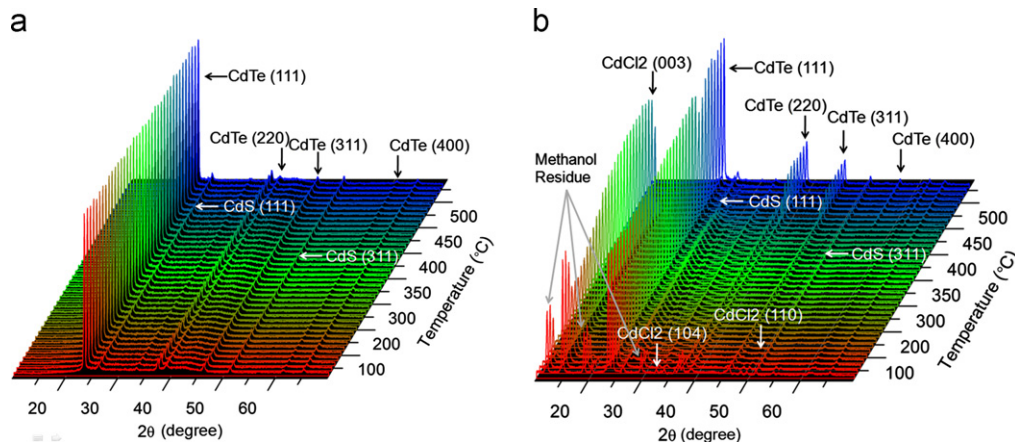


Fig. 1. In situ XRD scans during temperature ramp-up annealing of the Glass/FTO/CdS/CdTe sample (a) with and (b) without CdCl₂ treatment.

In this figure, the XRD peaks associated with the (003) rhombohedral CdCl₂ peak (a), (111) cubic CdTe peak (b and d), and (002) cubic CdTe peak (c) are shown. Fig. 2 shows graphically how the peak intensity and position changes as a function of heating temperature. Thermal expansion causes a decrease in the 2θ position, but the degree and behavior of the shift strongly depend on the presence of CdCl₂. By using data published in the literature [13] for the CdCl₂ vapor pressure, one can easily ascertain that in heating at temperatures from 100 to 125 °C, the vapor pressure (evaporation rate) of CdCl₂ increases by only $\sim 10^{-12}$, while between 375 and 400 °C, the increase in the vapor pressure (i.e., evaporation rate) is about 9 orders of magnitude greater ($\sim 10^{-3}$ increase). Therefore, the extinction of the CdCl₂ peak at about 400 °C is because there is no CdCl₂ left to diffract. Further quantitative explanation related to Fig. 2 will be discussed later.

Fig. 3 illustrates the quantitative XRD peak information of the Gaussian-fitted integrated areas associated with Fig. 2 as a function of the ramp annealing temperature. Fig. 3 implies that the integrated areas associated with the crystal planes of CdTe (220) do not change until the integrated area of the CdTe (111) peak attains its maximum value; that is, until the recrystallization of the CdTe (111) plane is complete. When the integrated area of CdTe (111) begins to decrease after 440 °C, at which point the integrated area is at a maximum, the integrated areas of (220) begin to increase. This result clearly confirms that the recrystallization of CdTe (111) and that of other planes such as (220) and (311) do not share any common temperature regions. In other words, after the crystal growth of the CdTe (111) plane was complete, other planes began to recrystallize, that is, randomized orientation occurred. In addition, all of these phase evolutions are strongly dependent on the change in the CdCl₂ peaks. It is clear that when the integrated area of the CdCl₂ (003) peak begins to show a significant drop at around 460 °C, the CdTe (220) peak shows a rapid increase and the CdTe (111) peak shows an apparent decrease.

Fig. 4(a–c) shows the quantitative XRD peak position (and corresponding d-spacing) as a function of annealing temperature associated with (a) the CdCl₂ (003) peak, (b) the CdTe (111) peak, and (c) the CdTe (220) peaks. In Fig. 4(a), the CdCl₂ (003) peak is shown both with and without CdS present, while in Fig. 4(b) and (c), the data is shown for cases with and without CdCl₂ and CdS. As shown in Fig. 4(a), the CdCl₂ (003) peak exhibits a large shift of the centrum toward a lower 2θ (higher d-spacing) with increasing temperature, regardless of the presence of CdS. The peak position shifts from 15.1° at 25 °C, to 14.9° at 450 °C. The variation appears to be linearly dependent on the ramp-up temperature. Parallel to this, as shown in Fig. 4(b) and (c), there is a similar decrease in the

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